N-Acetyl-3-acetoxy-10H-phenothiazine

Other names: Promethazine M (hydroxy-ring), acetylated
Inchi: InChI=1S/C16H13NO3S/c1-10(18)17-13-5-3-4-6-15(13)21-16-9-12(20-11(2)19)7-8-14(16
InchiKey: HEYNDDQURRWZFF-UHFFFAOYSA-N
Formula: C16H13NO3S
SMILES: CC(=O)Oc1ccc2c(c1)Sc1ccccc1N2C(C)=O
Mol. weight [g/mol]: 299.34
CAS: 99536-23-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.35		Crippen Method
logp	3.761		Crippen Method
mcvol	213.260	ml/mol	McGowan Method
rinpol	2550.00		NIST Webbook
rinpol	2550.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C99536239&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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